Distributionnally Robust Optimization & Statistical Learning

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- Mathematical modelling
 - ♦ The **cost** f_x of a decision **parametrized** by $x \in X$
 - ♦ depends on an **uncertain variable** $\xi \in \Xi$
- ▶ Why do we want **robustness** in practical applications?

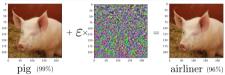
Difficult-to-predict environments



Biased, outdated, insufficient data

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Attacks against complex models



In phase with regulations



◊ Ben-Tal, Ghaoui, Nemirovski. Robust optimization. Princeton university press, 2009.

• Kolter, Madry. Adversarial robustness - theory and practice. NeurIPS tutorial https://adversarial-ml-tutorial.org/, 2018.

- Mathematical modelling
 - ♦ The **cost** f_x of a decision **parametrized** by $x \in X$
 - ♦ depends on an **uncertain variable** $\xi \in \Xi$
- ▶ Why do we want **robustness** in **statistical learning**?
 - ♦ cost = model + loss f_x on data point ξ ex. least squares $f_x(\xi = (a, b)) = (\langle x, a \rangle b)^2$
 - ♦ the uncertainty variable's **distribution** is known through samples $\xi_1, ..., \xi_N$
 - Robustness is desirable for
 - Generalization guarantees on the true distribution of the samples
 - ▶ Distribution shifts between training and application

▶ The uncertain variable ξ lives in some **uncertainty set** U

$$\min_{x \in \mathcal{X}} \sup_{\xi \in U} f_x(\xi)$$
 (Worst-case robustness)

- $\diamond U$ may be difficult to design
- pessimistic decisions (unlikely values of ξ)
- ▶ The uncertain variable ξ is known though its **empirical distribution** $\hat{\mathbf{P}}_N = \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i}$

 $\min_{x \in \mathcal{X}} \mathbb{E}_{\xi \sim \hat{\mathbf{P}}_N}[f_x(\xi)]$

(Sample Average Approximation)

- also called Empirical Risk Minimization in machine learning
- the empirical distribution $\hat{\mathbf{P}}_N$ may not be close to the true distribution of ξ in the target application too few samples, biased collection, distribution shifts
- ◊ Ben-Tal and Nemirovski. *Robust convex optimization*. Mathematics of operations research, 1998.
- Shapiro, Dentcheva, and Ruszczynski. Lectures on stochastic programming: modeling and theory. SIAM, 2021.

Distributionally Robust Optimization

- \triangleright The empirical distribution data provides **partial information** about the encountered **distribution** of ξ
 - \diamond The uncertain variable's **distribution** lives in a **neighborhood** $\mathcal{U}(\hat{\mathbf{P}}_N)$ of its empirical distribution

$$\min_{x \in \mathcal{X}} \sup_{\substack{\mathbf{Q} \in \mathcal{P}(\Xi) \\ \mathbf{Q} \in \mathcal{U}(\hat{\mathbf{P}}_{N})}} \mathbb{E}_{\boldsymbol{\xi} \sim \mathbf{Q}}[f_{x}(\boldsymbol{\xi})]$$
(DRO)

- Inner sup taken over the set $\mathcal{P}(\Xi)$ of probability measures on Ξ infinite dimensional
- For some U(P̂_N), parametric (Gaussian) or not (φ-divergences), this leads to finite-dimension min-max problems efficient stochastic optimization methods
- Enforces model robustness at training
- Scarf. A min-max solution of an inventory problem. Studies in the mathematical theory of inventory and production, 1958.
- ◊ Rahimian and Mehrotra. *Distributionally robust optimization: A review.* arXiv 1908.05659, 2019.
- Delage and Ye. Distributionally robust optimization under moment uncertainty with application to data-driven problems. Op. Res., 2010.
- Namkoong and Duchi. Stochastic gradient methods for distributionally robust optimization with f-divergences. NeurIPS, 2016.

Wasserstein Distributionally Robust Optimization

▶ The uncertain variable's **distribution** lives in a **Wasserstein neighborhood** of its empirical distribution

$$\min_{x \in \mathcal{X}} \sup_{\substack{\mathbf{Q} \in \mathcal{P}(\Xi) \\ W_{c}(\hat{\mathbf{P}}_{N}, \mathbf{Q}) \leq \rho}} \mathbb{E}_{\xi \sim \mathbf{Q}}[f_{x}(\xi)]$$
(WDRO)

• For a cost function $c: \Xi \times \Xi \to \mathbb{R}_+$, the Wasserstein distance between $\hat{\mathbf{P}}_N$ and \mathbf{Q} is defined as

$$W_c(\hat{\mathbf{P}}_N, \mathbf{Q}) = \inf \left\{ \mathbb{E}_{(\xi, \zeta) \sim \pi} \left[c(\xi, \zeta) \right] : \pi \in \mathcal{P}(\Xi \times \Xi), \pi_1 = \hat{\mathbf{P}}_N, \pi_2 = \mathbf{Q} \right\} \,,$$

with π_1 (resp. π_2) the first (resp. second) marginal of the transport plan π .

- **Natural metric** to compare empirical and absolutely continuous distributions contrary to the Kullback-Leibler divergence and strong generalization/concentration results
- Inner sup stays infinite dimensional and the constraint is itself linked to an optimization problem
- Esfahani and Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: performance guarantees and tractable reformulations. Mathematical Programming, 2018.
- Kuhn, Esfahani, Nguyen, and Shafieezadeh-Abadeh. Wasserstein distributionally robust optimization: Theory and applications in machine learning. In Operations Research & Management Science in the Age of Analytics, 2019.
- Blanchet and Murthy. Quantifying distributional model risk via optimal transport. Mathematics of Operations Research, 2019.
- Gao and Kleywegt. Distributionally robust stochastic optimization with Wasserstein distance. Mathematics of Operations Research, 2022.

- ▶ WDRO is an appealing framework for distributional robustness but difficult to optimize
 - ♦ Understand precisely the behavior of WDRO solutions
 - ♦ Study its statistical guarantees
 - Provide computationally tractable formulations for a large class of problems

Outline

Diving into the problem Statistical guarantees Approximation Optimization

Wasserstein Distributionally Robust Optimization

• Diving into the problem

- ▶ Let us investigate the WDRO inner problem (we drop the \min_x part)
 - ♦ Make explicit the Wasserstein constraint

$$\widehat{\mathcal{R}}_{\rho}(f_{x}) := \sup_{\substack{\mathbf{Q} \in \mathcal{P}(\Xi) \\ W_{c}(\widehat{\mathbf{P}}_{N}, \mathbf{Q}) \leq \rho}} \mathbb{E}_{\xi \sim \mathbf{Q}}[f_{x}(\xi)] \quad with \ W_{c}(\widehat{\mathbf{P}}_{N}, \mathbf{Q}) = \inf_{\substack{\pi \in \mathcal{P}(\Xi \times \Xi) \\ \pi_{1} = \widehat{\mathbf{P}}_{N}, \pi_{2} = \mathbf{Q}}} \mathbb{E}_{(\xi, \zeta) \sim \pi} \left[c(\xi, \zeta) \right]$$

Diving into the problem

- ▶ Let us investigate the WDRO inner problem (we drop the min_x part)
 - ♦ Make explicit the Wasserstein constraint Q disappears
 - ♦ Use the topological duality between signed measures and continuous functions on compact spaces

$$\widehat{\mathcal{R}}_{\rho}(f_{x}) \coloneqq \sup_{\substack{\mathbf{Q}\in\mathcal{P}(\Xi)\\W_{c}(\widehat{\mathbf{P}}_{N},\mathbf{Q})\leq\rho}} \mathbb{E}_{\xi\sim\mathbf{Q}}[f_{x}(\xi)] = \sup_{\substack{\pi\in\mathcal{P}(\Xi\times\Xi)\\\pi_{1}=\widehat{\mathbf{P}}_{N}, \ \mathbb{E}_{(\xi,\zeta)\sim\pi}[c(\xi,\zeta)]\leq\rho}} \mathbb{E}_{\zeta\sim\pi_{2}}\left[f_{x}(\zeta)\right]$$

Diving into the problem

- ▶ Let us investigate the WDRO inner problem (we drop the \min_x part)
 - ♦ Make explicit the Wasserstein constraint Q disappears
 - ♦ Use the topological duality between signed measures and continuous functions on compact spaces
 - ♦ Denoting by $\langle \cdot, \cdot \rangle$ the corresponding duality pairing so that $\langle \pi, \varphi \rangle \coloneqq \int_X \varphi(x) \, \mathrm{d} \pi(x)$ with $\tilde{f}_x : (\xi, \zeta) \mapsto f_x(\zeta)$ and *c* assumed to be continuous Riesz representation theorem

$$\widehat{\mathcal{R}}_{\rho}(f_{x}) \coloneqq \sup_{\substack{\mathbf{Q} \in \mathcal{P}(\Xi) \\ W_{c}(\widehat{\mathbf{P}}_{N}, \mathbf{Q}) \leq \rho}} \mathbb{E}_{\xi \sim \mathbf{Q}}[f_{x}(\xi)] = \sup_{\substack{\pi \in \mathcal{M}(\Xi \times \Xi) \\ \pi_{1} = \widehat{\mathbf{P}}_{N}, \ \langle \pi, c \rangle \leq \rho}} \langle \pi, \widetilde{f_{x}} \rangle$$

Diving into the problem

- ▶ Let us investigate the WDRO inner problem (we drop the \min_x part)
 - ♦ Make explicit the Wasserstein constraint Q disappears
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- > This is a **linear program** on measures
 - The solutions belong to the **border** of the constraint set
 - The optimal worst-case distribution π_2^* is supported on N + 1 atoms LP with N + 1 constraints
- ◇ Pinelis. On the extreme points of moments sets. Mathematical Methods of Operations Research, 2016.
- Yue, Kuhn, and Wiesemann. On linear optimization over Wasserstein balls. Mathematical Programming, 2021.

Dual problem

- **Duality** is at the core of modern WDRO
 - ♦ Lagrangian duality + Sup over (conditional) measure realized by a Dirac at the sup

$$\begin{aligned} \widehat{\mathcal{R}}_{\rho}(f_{x}) &= \sup_{\substack{\pi \in \mathcal{P}(\Xi \times \Xi) \\ \pi_{1} = \widehat{\mathbf{P}}_{N}, \ \mathbb{E}_{(\xi,\zeta) \sim \pi}[c(\xi,\zeta)] \leq \rho}} \mathbb{E}_{\zeta \sim \pi_{2}}\left[f_{x}(\zeta)\right] \\ &= \inf_{\lambda \geq 0} \lambda \rho + \mathbb{E}_{\xi \sim \widehat{\mathbf{P}}_{N}}\left[\sup_{\zeta \in \Xi} \left\{f_{x}(\zeta) - \lambda c(\xi,\zeta)\right\}\right] \end{aligned}$$
(Dual-WDRO)

- ▶ Main improvement: this is a finite-dimensional problem and λ is 1D!
 - If the sup is tractable, the Dual-WDRO problem is solvable! and thus WDRO, but that's a big if
 - ♦ The optimal **worst-case distribution** is supported on N + 1 atoms taken in $\arg \max_{\zeta \in \Xi} \{f_x(\zeta) \lambda^* c(\xi_i, \zeta)\}$ for i = 1, ..., N
- Esfahani and Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: Performance guarantees and tractable reformulations. Mathematical Programming, 2018.
- Zhao and Guan. Data-driven risk-averse stochastic optimization with Wasserstein metric. Operations Research Letters, 2018.
- Blanchet and Murthy. Quantifying distributional model risk via optimal transport. Mathematics of Operations Research, 2019.
- Gao and Kleywegt. Distributionally robust stochastic optimization with Wasserstein distance. Mathematics of Operations Research, 2022.
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(Dual) Optimization of WDRO problems

▶ Putting it all together, we have to solve

$$\min_{\substack{x \in \mathcal{X} \\ W_{c}(\hat{P}_{N}, \mathbf{Q}) \leq \rho}} \underbrace{\sup_{\substack{\xi \in \mathcal{P}(\Xi) \\ W_{c}(\hat{P}_{N}, \mathbf{Q}) \leq \rho}} \mathbb{E}_{\xi \sim \mathbf{Q}}[f_{x}(\xi)]}_{\mathbb{E}_{\xi \sim \mathbf{Q}}} = \min_{x \in \mathcal{X}} \inf_{\lambda \geq 0} \lambda \rho + \mathbb{E}_{\xi \sim \hat{\mathbf{P}}_{N}} \left[\sup_{\zeta \in \Xi} \left\{ f_{x}(\zeta) - \lambda c(\xi, \zeta) \right\} \right]$$

- ▶ min/min problem easier than previous min-max but with an inner sup bottleneck
- ▶ Strong interplay between the loss f_x and the transport cost *c*
 - ♦ With *x* fixed, λ should be such that $\sup_{\zeta \in \Xi} \{f_x(\zeta) \lambda c(\xi, \zeta)\} < +\infty$
 - $\diamond~$ If Ξ is bounded and the loss and cost are Lipschitz, this is ok
 - If Ξ is unbounded, $\frac{f_x(\zeta)}{c(\xi,\zeta)}$ should be uniformly bounded

Example I – the NewsVendor problem

- ▶ A NewsVendor has to decide how many papers he will buy for tomorrow
 - ♦ His buying price is k = 5 and his retail price is u = 7
 - ♦ He has a collection of sales data $\xi_1, ..., \xi_N$
 - ♦ He wants to minimize its loss $f_x(\xi) = kx u \min(x, \xi)$ by optimizing the number $x \in \mathbb{R}_+$ of newspaper bought, facing the uncertain demand of tomorrow $\xi \in \mathbb{R}_+$

- Taking a robust decision
 - Worst-case robustness leads to $x_{WCR}^{\star} = 0$ since $\xi = 0$ is possible
 - ♦ Sample Average Approximation leads to $x_{SAA}^{\star} > 0$ by minimizing the average loss over the past
 - ♦ What about WDRO?

Example I - the NewsVendor problem

- ▶ A NewsVendor has to decide how many papers he will buy for tomorrow
 - ♦ His buying price is k = 5 and his retail price is u = 7
 - ♦ He has a collection of sales data $\xi_1, ..., \xi_N$ in $\mathbb{R}_+ = \Xi$
 - ♦ He wants to minimize its loss $f_x(\xi) = kx u \min(x, \xi)$ by optimizing the number $x \in \mathbb{R}_+$ of newspaper bought, facing the uncertain demand of tomorrow $\xi \in \mathbb{R}_+$

$$\min_{x\geq 0} \inf_{\lambda\geq 0} \lambda \rho + \frac{1}{N} \sum_{i=1}^{N} \sup_{\zeta\in\Xi} \left\{ kx - u \min(x,\zeta) - \lambda |\xi_i - \zeta| \right\}$$

- ▶ We can solve Dual-WDRO with $c(\xi, \zeta) = |\xi \zeta|$
 - If $\lambda^* = 0$, the sup is attained at $\zeta_i^* = 0$ for all ξ_i , leading to $x^* = 0 \rightarrow \rho$ too large, worst-case
 - If $\lambda^* \geq u$, the sup is attained at $\zeta_i^* = \xi_i$ for each $\xi_i \rightarrow SAA$ problem linear cost/function cancel out
 - ♦ $\lambda \in (0, u)$ cannot be optimal gradient either positive or negative
- ▶ WDRO leads to $x_{WCR}^{\star} = 0$ or x_{SAA}^{\star} depending on ρ !

- Standard classification problem
 - ♦ Labeled data $\xi_1, ..., \xi_N$ of the form $\xi_i = (x_i, y_i) \in \mathbb{R}^d \times \{-1, +1\} = \Xi$
 - We minimize the loss $f_x(\xi = (x', y')) = \log(1 + \exp(-y'\langle x', x \rangle))$ by fitting separator $x \in \mathbb{R}^d$

$$\min_{x \in \mathbb{R}^d} \inf_{\lambda \ge 0} \lambda \rho + \frac{1}{N} \sum_{i=1}^N \sup_{\zeta = (z, \nu) \in \Xi} \left\{ \log(1 + \exp(-y_i \langle x_i, x \rangle)) - \lambda \left(\|x_i - z\| + \kappa \mathbb{1}_{y_i \neq \nu} \right) \right\}$$

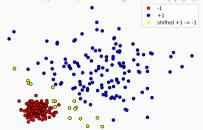
▶ We can solve Dual-WDRO by disciplined convex programming

• for this, $c(\xi = (x, y), \zeta = (z, v)) = ||x - z|| + \kappa \mathbb{1}_{y \neq v}$ if $\kappa = +\infty$, (WDRO) is ERM regularized by $\rho ||x||_*$

$$\min_{x,\lambda,s} \quad \lambda \rho + \frac{1}{N} \sum_{i=1}^{N} s_i$$
s.t.
$$\log(1 + \exp(-y_i \langle x_i, x \rangle)) \le s_i \ \forall i$$

$$\log(1 + \exp(y_i \langle x_i, x \rangle)) - \kappa \lambda \le s_i \ \forall i$$

$$\|x\|_* \le \lambda$$



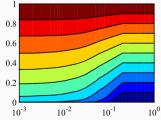
Example III – Portfolio selection

- ▷ Optimize a portfolio $x \in \{y \in \mathbb{R}^d_+ : \sum_{i=1}^d y[i] = 1\}$ over *m* assets subject to uncertain yearly returns
 - ♦ Return data $\xi_1, ..., \xi_N$ in $\mathbb{R}^d = \Xi$
 - We minimize a risk-averse loss $f_x(\xi, \tau) = -\langle x, \xi \rangle + \eta \tau + \frac{\eta}{\alpha} \max(-\langle x, \xi \rangle \tau; 0)$ with $\eta \ge 0$ is the risk aversion and $\alpha \in (0, 1]$ is the risk level \rightsquigarrow risk $\mathbb{E}[-\langle x, \xi \rangle] + \eta \operatorname{CVaR}_{\alpha}[-\langle x, \xi \rangle]$

$$\min_{x \in \{\mathbb{R}^d_+: \sum_{i=1}^d x[i]=1\}} \min_{\tau \in \mathbb{R}} \inf_{\lambda \ge 0} \lambda \rho + \frac{1}{N} \sum_{i=1}^N \sup_{\zeta \in \Xi} \left\{ -\langle x, \zeta \rangle + \eta \tau + \frac{\eta}{\alpha} \max(-\langle x, \zeta \rangle - \tau; 0) - \lambda \|\xi_i - \zeta\| \right\}$$

▶ We can again solve Dual-WDRO by disciplined convex programming for $c(\xi, \zeta) = \|\xi - \zeta\|$

$$\begin{split} \min_{x,\tau,\lambda,s} & \lambda \rho + \frac{1}{N} \sum_{i=1}^{N} s_i \\ \text{s.t.} & \eta \tau - \langle x, \xi_i \rangle \leq s_i \quad \forall i \\ & \eta (1 - 1/\alpha) \tau - (1 + \eta/\alpha) \langle x, \xi_i \rangle \leq s_i \quad \forall i \\ & \|x\|_* \leq \lambda/\eta, \sum_{i=1}^d x[i] = 1, x \geq 0 \end{split}$$



Portfolio as a function of ρ Source: Esfahani & Kuhn, 2018 1

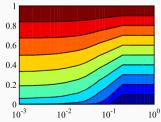
Example III – Portfolio selection

x

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$$\min_{\epsilon \in \{\mathbb{R}^d_+: \sum_{i=1}^d x[i]=1\}} \min_{\tau \in \mathbb{R}} \inf_{\lambda \ge 0} \lambda \rho + \frac{1}{N} \sum_{i=1}^N \sup_{\zeta \in \Xi} \left\{ -\langle x, \zeta \rangle + \eta \tau + \frac{\eta}{\alpha} \max(-\langle x, \zeta \rangle - \tau; 0) - \lambda \|\xi_i - \zeta\| \right\}$$

- ▶ We can again solve Dual-WDRO by disciplined convex programming for $c(\xi, \zeta) = \|\xi \zeta\|$
- Recovers that optimality of equally weighted portfolio under high ambiguity
- Esfahani and Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: Performance guarantees and tractable reformulations. Mathematical Programming, 2018.
- Pflug, Pichler, Wozabal. The 1/N investment strategy is optimal under high model ambiguity. J. Bank. Financ., 2012.
- Rockafellar and Uryasev. Optimization of conditional value-at-risk. J. Risk, 2000.



Portfolio as a function of ρ Source: Esfahani & Kuhn, 2018

Wasserstein Distributionally Robust Optimization

Statistical guarantees

Statistical properties of WDRO: a first approach

- ▶ Let $\hat{\mathbf{P}}_N = \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i}$ with $\xi_i \sim \mathbf{P}$ i.i.d.
 - ♦ We can see **P** as the *true* distribution encountered in practice
 - ♦ Take $c(\xi, \zeta) = \|\xi \zeta\|^2$ and $\Xi \subset \mathbb{R}^d$ compact, convex, with nonempty interior
 - Concentration results for optimal transport P has finite moments

$$\mathbb{P}\left[W_2^2(\hat{\mathbf{P}}_N, \mathbf{P}) \le \rho^2\right] \ge 1 - c_1 e^{-c_2 N \rho^d}$$

• With probability at least $1 - \delta$, taking $\rho \propto \frac{\log(1/\delta)}{N^{1/d}}$, for any f_x

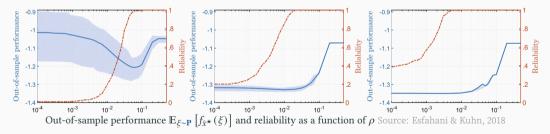
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$$\mathbb{E}_{\xi \sim \mathbf{P}}[f_x(\xi)] \leq \widehat{\mathcal{R}}_{\rho}(f_x) = \sup_{\substack{\mathbf{Q} \in \mathcal{P}(\Xi) \\ W_2(\widehat{\mathbf{P}}_N, \mathbf{Q}) \leq \rho}} \mathbb{E}_{\xi \sim \mathbf{Q}}[f_x(\xi)]$$
 computable

♦ Overly pessimistic due to the curse of dimensionality *N* scales exponentially in *d*

- Fournier and Guillin. On the rate of convergence in Wasserstein distance of the empirical measure. Probability Theory and Related Fields, 2015
- Esfahani and Kuhn. Data-driven distributionally robust optimization using the Wasserstein metric: performance guarantees and tractable reformulations. Mathematical Programming, 2018.

Statistical properties of WDRO: illustration on Example III - Portfolio selection

- Sample 200 training datasets of size $N = \{30, 300, 3000\}$ from the same distribution
 - for each of them, solve WDRO to get optimal point \hat{x}^{\star} and value $\widehat{\mathcal{R}}_{\rho}(f_{\hat{x}^{\star}})$
- ▶ **Reliability** = pc. of datasets s.t. the WDRO value is greater than the loss at the WDRO optimal point: estimated by taking N = 30000 target $\mathbb{E}_{\xi \sim \mathbf{P}} [f_{\hat{x}^{\star}}(\xi)] \leq \widehat{\mathcal{R}}_{\rho}(f_{\hat{x}^{\star}})$ computed



▶ To get a fixed reliability, no need to scale $\frac{1}{N^{1/10}}$, $\frac{1}{\sqrt{N}}$ seems enough!

Statistical properties of WDRO: a finer proposition

- ▶ **Objective:** Get that with high probability $\mathbb{E}_{\xi \sim \mathbf{P}} [f_x(\xi)] \leq \widehat{\mathcal{R}}_{\rho}(f_x)$
- ▶ Why can we hope to do better than measure concentration ?
 - We do no *need* to bound the distance $W_2^2(\hat{\mathbf{P}}_N, \mathbf{P})$ whp.
 - ♦ Using the dual formulation, we can reformulate the target inequality as

$$\begin{split} \mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{P}}\left[f_{\boldsymbol{x}}\left(\boldsymbol{\xi}\right)\right] &= \sup_{\substack{\mathbf{Q}\in\mathcal{P}(\Xi)\\W_{2}(\mathbf{P},\mathbf{Q})\leq0}} \mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{Q}}\left[f_{\boldsymbol{x}}\left(\boldsymbol{\xi}\right)\right] \\ &= \inf_{\boldsymbol{\lambda}\geq0} \mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{P}}\left[\sup_{\boldsymbol{\zeta}\in\Xi}\left\{f_{\boldsymbol{x}}\left(\boldsymbol{\zeta}\right)-\boldsymbol{\lambda}\|\boldsymbol{\xi}-\boldsymbol{\zeta}\|^{2}\right\}\right] &\leq \inf_{\boldsymbol{\lambda}\geq0}\boldsymbol{\lambda}\rho + \mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{P}_{\mathbf{N}}}\left[\sup_{\boldsymbol{\zeta}\in\Xi}\left\{f_{\boldsymbol{x}}\left(\boldsymbol{\zeta}\right)-\boldsymbol{\lambda}\|\boldsymbol{\xi}-\boldsymbol{\zeta}\|^{2}\right\}\right] \\ &= \widehat{\mathcal{R}}_{\rho}(f_{\boldsymbol{x}}) \end{split}$$

♦ *Rather*, we may show that whp uniformly in f_x (ok...) and in λ (less cool)

$$\frac{\mathbb{E}_{\xi \sim \mathbf{P}} \left[\sup_{\zeta \in \Xi} \left\{ f_x(\zeta) - \lambda \| \xi - \zeta \|^2 \right\} \right]}{\lambda} \leq \frac{\mathbb{E}_{\xi \sim \hat{\mathbf{P}}_N} \left[\sup_{\zeta \in \Xi} \left\{ f_x(\zeta) - \lambda \| \xi - \zeta \|^2 \right\} \right]}{\lambda} + \rho$$

The concentration error is directly related to the radius ρ hopefully with a good dependency in N...

Concentration

▶ For $\delta \in (0, 1)$ and some $0 < \frac{\lambda}{2} < +\infty$, we have with probability at least $1 - \delta/2$ that

$$\sup_{\substack{(f_x,\lambda)\in\mathcal{F}\times[\underline{\lambda},+\infty)}} \left\{ \frac{\mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{P}} \left[\sup_{\boldsymbol{\zeta}\in\Xi} \left\{ f_x(\boldsymbol{\zeta}) - \lambda \|\boldsymbol{\xi} - \boldsymbol{\zeta}\|^2 \right\} \right] - \mathbb{E}_{\boldsymbol{\xi}\sim\hat{\mathbf{P}}_N} \left[\sup_{\boldsymbol{\zeta}\in\Xi} \left\{ f_x(\boldsymbol{\zeta}) - \lambda \|\boldsymbol{\xi} - \boldsymbol{\zeta}\|^2 \right\} \right]}{\lambda} \right\} \\ \leq \frac{117}{\sqrt{N}\underline{\lambda}} \left(\mathcal{I}(\mathcal{F}) + \operatorname{Cst} \left(1 + \sqrt{\log\frac{1}{\delta}} \right) \right) := \rho_N$$

- Error \leftrightarrow minimal radius for concentration in $O\left(\frac{1}{\sqrt{N}}\right)$ no curse of dimension
- The complexity of the class of functions appears as one can expect
- Lower bound on the dual variable, λ, needed we have to show it
- ▶ Proof relies on standard concentration results + sup Lipschitz and bounded
- Boucheron, Lugosi, and Massart. Concentration Inequalities. A Nonasymptotic Theory of Independence. Oxford University Press, 2013.

Lower-bounding the dual variable

▶ Crux of the proof for getting the concentration result: if $\lambda > \lambda$, we have with probability $1 - \delta/2$

 $\mathbb{E}_{\xi \sim \mathbf{P}}\left[f_x(\xi)\right] \leq \widehat{\mathcal{R}}_{\rho}(f_x)$

whenever ρ is bigger than $\rho_N = \frac{117}{\sqrt{N\lambda}} \left(I(\mathcal{F}) + \operatorname{Cst} \left(1 + \sqrt{\log \frac{1}{\delta}} \right) \right)$.

- ▷ Careful analysis of the dual function: It's all a matter of compromises
 - If ρ is small, the constraint is stringent, λ is big BUT ρ has to be also greater than ρ_N
 - If ρ is bigger, we have more margin for error
 BUT the constraint has to be sufficiently active so that λ does not vanish
 - The lower bound depends on P̂_N natively which is not nice
 SO we also need to concentrate the opposite quantity to get back to P
 - ♦ AND the minimal λ depends on ρ ...

Theorem (Azizian, I., Malick'23 – informal) *There is a critical radius* ρ_c *depending only on* \mathcal{F} *and* \mathbf{P} *such that for any* $\delta \in (0, 1)$ *and* $N \ge 1$, *if*

$$O\left(\sqrt{\frac{1+\log 1/\delta}{N}}\right) \le \rho \le \frac{\rho_c}{2} - O\left(\sqrt{\frac{1+\log 1/\delta}{N}}\right)$$

then, there is $\rho_N = O\left(\sqrt{\frac{1+\log 1/\delta}{N}}\right)$ such that, with probability $1 - \delta$, $\forall f_x \in \mathcal{F}$, $\mathbb{E}_{\xi \sim \mathbf{Q}}\left[f_x(\xi)\right] \leq \widehat{\mathcal{R}}_{\rho}(f_x) \quad \text{for all } \mathbf{Q} \text{ such that } W_2(\mathbf{P}, \mathbf{Q}) \leq \sqrt{\rho(\rho - \rho_N)},$

In particular, with probability $1 - \delta$, we have $\forall f_x \in \mathcal{F}$,

 $\mathbb{E}_{\boldsymbol{\xi}\sim\mathbf{P}}\left[f_{\boldsymbol{x}}(\boldsymbol{\xi})\right] \leq \widehat{\mathcal{R}}_{\rho}(f_{\boldsymbol{x}}).$

▷ $\rho_c = \sqrt{\inf_{f_x \in \mathcal{F}} \mathbb{E}_{\xi \sim \mathbf{P}} \left[\frac{1}{2} d^2(\xi, \arg \max f_x) \right]}$ is the maximal radius before falling back to worst case robustness

- ▶ Assumptions
 - $\diamond~$ Sample space $\Xi~compact~convex$ + supp~P strictly included in Ξ with some margin
 - \diamond All functions f_x are twice differentiable + bounded/smooth regularized or non-convex models are ok
 - Decrease condition around maximizers of f_x uniformly + non-vanishing gradients ok for most linear models
- ▶ Literature: Bridging the gap between several results on concentration for WDRO with $\rho \propto 1/\sqrt{N}$
 - ♦ With error terms
 - ♦ Asymptotic
 - ◊ Experimental
- ◊ An and Gao. Generalization Bounds for (Wasserstein) Robust Optimization. NeurIPS, 2021.
- Blanchet, Murthy, and Si. Confidence regions in wasserstein distributionally robust estimation. Biometrika, 2022.

- ▶ WDRO models control the true risk with high probability
 - $\diamond\,$ Radius $\rho\,$ should be taken proportional to $1/\sqrt{N}$
 - \diamond Uniform in the model f_x we still have to optimize it!
- ▶ What about tightness?
 - ◇ Under the same assumptions whp.

$$\mathcal{R}_{\sqrt{\rho(\rho-\rho_N)}}(f_x) \le \widehat{\mathcal{R}}_{\rho}(f_x) \le \mathcal{R}_{\sqrt{\rho(\rho+\rho_N)}}(f_x)$$

with $\mathcal{R}_{\rho}(f_x)$ the (regularized) WDRO risk rooted at **P**

Wasserstein Distributionally Robust Optimization

♦ Approximation

Entropic regularization

- ▶ We wish to get rid of the **linearity** of the problem
 - ♦ We draw inspiration from regularization in optimal transport

WDRO

$$\begin{split} \sup_{\mathbf{Q}\in\mathcal{P}(\Xi)} & \mathbb{E}_{\xi\sim\mathbf{Q}}[f_x(\xi)] \\ W_c(\hat{\mathbf{P}}_{N,\mathbf{Q}}) \leq \rho \\ &= \inf_{\lambda\geq 0} \lambda\rho + \mathbb{E}_{\xi\sim\hat{\mathbf{P}}_N} \left[\sup_{\zeta\in\Xi} \left\{ f_x(\zeta) - \lambda c(\xi,\zeta) \right\} \right] \\ &\coloneqq \widehat{\mathcal{R}}_\rho(f_x) \end{split}$$

- ◊ Peyré, Cuturi. Computational Optimal Transport. Foundation and Trends in Machine Learning, 2019.
- ◊ Wang, Gao, and Xie. Sinkhorn Distributionally Robust Optimization. ArXiv 2109.11926, 2021.
- ◊ Azizian, I., Malick. Regularization for Wasserstein Distributionally Robust Optimization. ESAIM:COCV, 2022.
- Piat, Fadili, Jurie, da Veiga. Regularized Robust Optimization with Application to Robust Learning. preprint, 2022.

Entropic regularization

- We wish to get rid of the **linearity** of the problem
 - ♦ We draw inspiration from regularization in optimal transport

 $\begin{array}{ccc} \textbf{WDRO} & \textbf{Regularized WDRO} \\ \sup_{\substack{\pi \in \mathcal{M}(\Xi \times \Xi) \\ \pi_1 = \hat{\mathbf{P}}_N, \ \langle \pi, c \rangle \leq \rho \\ = & \inf_{\lambda \geq 0} \lambda \rho + \mathbb{E}_{\xi \sim \hat{\mathbf{P}}_N} \left[\sup_{\substack{\zeta \in \Xi}} \left\{ f_x(\zeta) - \lambda c(\xi, \zeta) \right\} \right] & := \widehat{\mathcal{R}}_{\rho}^{\ell}(f_x) \\ \end{array}$

• π must be absolutely continuous wrt. to the *chosen* π_0 and $(\pi_0)_1 = \hat{\mathbf{P}}_N$

- ◊ Peyré, Cuturi. Computational Optimal Transport. Foundation and Trends in Machine Learning, 2019.
- ◊ Wang, Gao, and Xie. Sinkhorn Distributionally Robust Optimization. ArXiv 2109.11926, 2021.
- Azizian, I., Malick. Regularization for Wasserstein Distributionally Robust Optimization. ESAIM:COCV, 2022.
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Entropic regularization

- We wish to get rid of the **linearity** of the problem
 - ♦ We draw inspiration from regularization in optimal transport

$\begin{array}{ccc} \textbf{WDRO} & \textbf{Regularized WDRO} \\ \sup_{\pi \in \mathcal{M}(\Xi \times \Xi)} & \langle \pi, \tilde{f}_x \rangle & \sup_{\pi \in \mathcal{M}(\Xi \times \Xi)} & \langle \pi, \tilde{f}_x \rangle & -\varepsilon \operatorname{KL}(\pi \mid \pi_0) \\ \pi_1 = \hat{\mathbf{P}}_N, \langle \pi, c \rangle \leq \rho & \pi_1 = \hat{\mathbf{P}}_N, \langle \pi, c \rangle \leq \rho \\ = \inf_{\lambda \geq 0} \lambda \rho + \mathbb{E}_{\xi \sim \hat{\mathbf{P}}_N} \left[\sup_{\zeta \in \Xi} \left\{ f_x(\zeta) - \lambda c(\xi, \zeta) \right\} \right] & = \inf_{\lambda \geq 0} \lambda \rho + \varepsilon \operatorname{E}_{\xi \sim \hat{\mathbf{P}}_N} \left[\log \left(\mathbb{E}_{\zeta \sim \pi_0(\cdot \mid \xi)} \left[e^{\frac{f_x(\zeta) - \lambda c(\xi, \zeta)}{\varepsilon}} \right] \right) \right] \\ \coloneqq \widehat{\mathcal{R}}_\rho(f_x) & \coloneqq \widehat{\mathcal{R}}_\rho^\varepsilon(f_x) \end{array}$

• π must be absolutely continuous wrt. to the *chosen* π_0 and $(\pi_0)_1 = \hat{\mathbf{P}}_N$

- Lagrangian then Fenchel duality in the space of finite signed measures on a compact space
- $\diamond~$ The \sup is transformed into a log-integral-exp
- ◊ Peyré, Cuturi. Computational Optimal Transport. Foundation and Trends in Machine Learning, 2019.
- ◊ Wang, Gao, and Xie. Sinkhorn Distributionally Robust Optimization. ArXiv 2109.11926, 2021.
- Azizian, I., Malick. Regularization for Wasserstein Distributionally Robust Optimization. ESAIM:COCV, 2022.
- Piat, Fadili, Jurie, da Veiga. Regularized Robust Optimization with Application to Robust Learning. preprint, 2022.

Approximation error

- ▶ The reference coupling π_0 is a kind of prior
 - In optimal transport, entropic regularization with $KL(\pi | \mathbf{P} \otimes \mathbf{Q}) \pi_0$ is the product of marginals
 - ♦ In WDRO, the second marginal is **not fixed** but optimized to get our adversarial distribution
 - $\diamond \text{ We choose } \pi_0(\mathrm{d}\xi,\mathrm{d}\zeta) \propto \hat{\mathbf{P}}_N(\mathrm{d}\xi) e^{-\frac{\|\xi-\zeta\|^p}{2^{p-1}\sigma}} \mathbbm{1}_{\zeta \in \Xi} \mathrm{d}\zeta$

$$\begin{split} \widehat{\mathcal{R}}_{\rho}(f_{x}) &= \inf_{\lambda \geq 0} \lambda \rho + \mathbb{E}_{\xi \sim \widehat{\mathbf{P}}_{N}} \left[\sup_{\zeta \in \Xi} \left\{ f_{x}(\zeta) - \lambda \| \xi - \zeta \|^{p} \right\} \right] \tag{WDRO} \\ \widehat{\mathcal{R}}_{\rho}^{\varepsilon}(f_{x}) &= \inf_{\lambda \geq 0} \lambda \rho + \varepsilon \mathbb{E}_{\xi \sim \widehat{\mathbf{P}}_{N}} \left[\log \left(\mathbb{E}_{\zeta \sim \pi_{0}}(\cdot |\xi) \left[e^{\frac{f_{x}(\zeta) - \lambda \| \xi - \zeta \|^{p}}{\varepsilon}} \right] \right) \right] \tag{WDRO} \end{split}$$

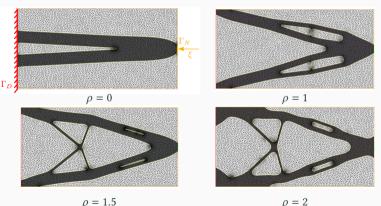
Theorem (Azizian, I., Malick'22) If $\Xi \subset \mathbb{R}^d$ is compact, convex, with nonempty interior and f_x is Lipschitz continuous, then as ε goes to 0

$$0 \le \widehat{\mathcal{R}}_{\rho}(f_x) - \widehat{\mathcal{R}}_{\rho}^{\varepsilon}(f_x) \le O\left(\varepsilon d \log\left(\frac{1}{\varepsilon}\right)\right)$$

[◊] Genevay, Chizat, Bach, Cuturi, and Peyré. Sample complexity of sinkhorn divergences. AIStats, 2019.

Example IV – A problem that has no tractable WDRO formulation

- > Optimization of a cantilever beam minimization of the compliance under a volume constraint
 - ♦ Uncertainty lies in the load ξ applied around the vector (-1, 0)
- ▶ Entropic WDRO formulation over a finite element solver Expectation approx. by a 10 Gaussian samples



 Dapogny, I., Meda, Thibert. Entropy-regularized Wasserstein distributionally robust shape and topology optimization. Structural and Multidisciplinary Optimization, ArXiv 2209.01500, 2022.

- ▶ Thanks to our duality results, we can use the same kind of technique
 - ♦ Classical

$$\frac{\mathbb{E}_{\boldsymbol{\xi} \sim \mathbf{P}} \left[\sup_{\boldsymbol{\zeta} \in \Xi} \left\{ f_x(\boldsymbol{\zeta}) - \lambda \| \boldsymbol{\xi} - \boldsymbol{\zeta} \|^2 \right\} \right]}{\lambda} \leq \frac{\mathbb{E}_{\boldsymbol{\xi} \sim \hat{\mathbf{P}}_N} \left[\sup_{\boldsymbol{\zeta} \in \Xi} \left\{ f_x(\boldsymbol{\zeta}) - \lambda \| \boldsymbol{\xi} - \boldsymbol{\zeta} \|^2 \right\} \right]}{\lambda} + \rho$$

• **Regularized** with
$$-\varepsilon \operatorname{KL}(\pi | \pi_0)$$
 and $\pi_0(d\xi, d\zeta) \propto \hat{\mathbf{P}}_N(d\xi) e^{-\frac{\|\xi-\zeta\|^2}{2\sigma}} \mathbb{1}_{\zeta \in \Xi} d\zeta$

$$\frac{\varepsilon \mathbb{E}_{\boldsymbol{\xi} \sim \mathbf{P}} \left[\log \left(\mathbb{E}_{\boldsymbol{\zeta} \sim \pi_0(\cdot | \boldsymbol{\xi})} \left[e^{\frac{f_{\boldsymbol{\chi}}(\boldsymbol{\zeta}) - \lambda \| \boldsymbol{\xi} - \boldsymbol{\zeta} \|^2}{\varepsilon}} \right] \right) \right]}{\lambda} \leq \frac{\varepsilon \mathbb{E}_{\boldsymbol{\xi} \sim \hat{\mathbf{P}}_N} \left[\log \left(\mathbb{E}_{\boldsymbol{\zeta} \sim \pi_0(\cdot | \boldsymbol{\xi})} \left[e^{\frac{f_{\boldsymbol{\chi}}(\boldsymbol{\zeta}) - \lambda \| \boldsymbol{\xi} - \boldsymbol{\zeta} \|^2}{\varepsilon}} \right] \right) \right]}{\lambda} + \rho$$

- Same proof layout but quite different derivations
 - The additional parameters ε and σ should be taken proportional to ρ to get close to the true risk at the same time it naturally appears in the proofs

then.

Theorem (Azizian, I., Malick'23 – informal)

For $\sigma = \sigma_0 \rho$ with $\sigma_0 > 0$, $\varepsilon = \varepsilon_0 \rho$ with $\varepsilon_0 > 0$ such that $\varepsilon_0 / \sigma_0^2$ is small enough depending on \mathcal{F} , \mathbf{P} , Ξ , there is an explicit constant ρ_c depending only on \mathcal{F} , \mathbf{P} and Ξ such that for all $\delta \in (0, 1)$ and $N \ge 1$, if

$$O\left(\sqrt{\frac{1+\log 1/\delta}{N}}\right) \le \rho \le \frac{\rho_c}{2} - O\left(\frac{1}{\sqrt{N}}\right), \quad and \quad \rho_c \ge O\left(\frac{1}{N^{1/6}} + \left(\frac{1+\log 1/\delta}{N}\right)^{1/4}\right),$$

there are $\tau = O(\varepsilon\rho)$ and $\rho_N = O\left(\sqrt{\frac{1+\log 1/\delta}{N}}\right)$ such that, with probability at least $1 - \delta$, $\forall f_x \in \mathcal{F}$,

 $\mathbb{E}_{\xi \sim \mathbf{Q}} \left[f_x(\xi) \right] \leq \widehat{\mathcal{R}}_{\rho}^{\varepsilon}(f_x) \qquad \text{for all } \mathbf{Q} \text{ such that } W_{2,\tau}(\mathbf{P}, \mathbf{Q}) \leq \sqrt{\rho(\rho - \rho_N)}$

Furthermore, when σ_0 and σ are small enough depending on **P** and Ξ , with probability $1 - \delta$, $\forall f_x \in \mathcal{F}$,

$$\mathbb{E}_{\xi \sim \mathbf{P}} \mathbb{E}_{\zeta \sim \pi_0(\cdot|\xi)} \left[f_x(\zeta) \right] \le \widehat{\mathcal{R}}_{\rho}^{\varepsilon}(f_x).$$

- ▶ Not exactly an upper bound on the true risk on **P** but rather the risk for smoothed **P** * $\pi_0(\cdot|\xi)$
- $\blacktriangleright \quad \text{Robust wrt. } W_{2,\tau}(\mathbf{P},\mathbf{Q}) \coloneqq \sqrt{\inf \left\{ \mathbb{E}_{\pi} \left[\frac{1}{2} \| \xi \zeta \|^2 \right] + \tau \operatorname{KL}(\pi \mid \pi_0) : \pi \in \mathcal{P}(\Xi \times \Xi), \pi_1 = \mathbf{P}, \ \pi_2 = \mathbf{Q} \right\}}$

▶ The WDRO problem $\widehat{\mathcal{R}}_{\rho}(f_x)$ can be controllably approximated by

$$\widehat{\mathcal{R}}^{\varepsilon}_{\rho}(f_{x}) = \sup_{\substack{\pi \in \mathcal{M}(\Xi \times \Xi) \\ \pi_{1} = \widehat{\mathbf{P}}_{N, \ \langle \pi, c \rangle \leq \rho}} \langle \pi, \tilde{f}_{x} \rangle -\varepsilon \operatorname{KL}(\pi \mid \pi_{0}) = \inf_{\lambda \geq 0} \lambda \rho + \varepsilon \operatorname{\mathbb{E}}_{\xi \sim \widehat{\mathbf{P}}_{N}} \left[\log \left(\operatorname{\mathbb{E}}_{\zeta \sim \pi_{0}}(\cdot \mid \xi) \left[e^{\frac{f_{x}(\zeta) - \lambda \|\xi - \zeta\|^{p}}{\varepsilon}} \right] \right) \right]$$

- ♦ Differentiable and more tractable problem as soon as the inner integral can be evaluated
- ▶ This is not exactly a Sinkhorn distance
 - ♦ We can regularize in the objective and/or in the constraints
 - ♦ We cannot symmetrize to get an actual distance
- ▶ Worst case probability measures from optimal dual value λ^*

$$\propto \sum_{i=1}^{N} e^{\frac{f_{\mathcal{X}}(\zeta) - \lambda^{\star} \|\xi_i - \zeta\|^p}{\varepsilon}} e^{-\frac{\|\xi_i - \zeta\|^p}{2^{p-1}\sigma}} \, 1\!\!\!1_{\zeta \in \Xi} \, \mathrm{d}\zeta$$

- ▶ Concentration is very similar for the regularized version
 - ♦ Insight on the choice of $\varepsilon \propto \rho$ same thing for σ
 - Thanks to regularization, we get rid of the need to control the behavior near maximizers

Wasserstein Distributionally Robust Optimization

Optimization

Solving generic WDRO problems

▶ Leverage the entropic regularization

$$\min_{x \in \mathcal{X}} \inf_{\lambda \ge 0} \lambda \rho + \varepsilon \frac{1}{N} \sum_{i=1}^{N} \left[\log \left(\mathbb{E}_{\zeta \sim \pi_0}(\cdot |\xi_i) \left[e^{\frac{f_x(\zeta) - \lambda \|\xi_i - \zeta\|^2}{\varepsilon}} \right] \right) \right]$$

♦ Gradients in *x* and λ are available

$$\frac{1}{N}\sum_{i=1}^{N}\left[\frac{\mathbb{E}_{\zeta\sim\pi_{0}}(\cdot|\xi_{i})\nabla_{x}f_{x}(\zeta)e^{\frac{f_{x}(\zeta)-\lambda||\xi_{i}-\zeta||^{2}}{\varepsilon}}}{\mathbb{E}_{\zeta\sim\pi_{0}}(\cdot|\xi_{i})e^{\frac{f_{x}(\zeta)-\lambda||\xi_{i}-\zeta||^{2}}{\varepsilon}}}\right] \text{ and } \rho-\frac{1}{N}\sum_{i=1}^{N}\left[\frac{\mathbb{E}_{\zeta\sim\pi_{0}}(\cdot|\xi_{i})|\xi_{i}-\zeta||^{2}e^{\frac{f_{x}(\zeta)-\lambda||\xi_{i}-\zeta||^{2}}{\varepsilon}}}{\mathbb{E}_{\zeta\sim\pi_{0}}(\cdot|\xi_{i})e^{\frac{f_{x}(\zeta)-\lambda||\xi_{i}-\zeta||^{2}}{\varepsilon}}}\right]$$

- ▷ **Crude approach:** sample some points from $\pi_0(\cdot|\xi_i) \propto e^{\frac{\|\xi_i \zeta\|^2}{2\sigma}} \mathbb{1}_{\zeta \in \Xi}$ and minimize the sampled loss
 - $\diamond~$ This is a biased approximation with poor performance in practice except for d=1
- ▶ Better approach: sample the expectation at each iteration by (Metropolis-adjusted) Langevin
 - \diamond "Robustifies" but unstable behavior of λ
- ▶ **Implemented approach:** additionally use importance sampling towards $\nabla_{\xi_i} f_x(\xi_i)$
 - $\diamond\,$ Much more stable, when initialized with the ERM solution

Talking code

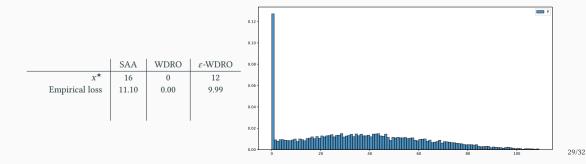
- Python package coming soon Two modes:
 - ♦ <u>à la scikit-learn</u>

from sklearn.linear_model import LogisticRegression # scikit-learn's standard version
from skwdro.linear_models import LogisticRegression as WDROLogisticRegression # WDRO version

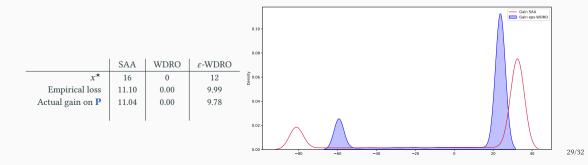
◊ à la pytorch

```
from typing import Optional
from abc import abstractclassmethod, abstractproperty
import torch as pt
import torch.nn as nn
    """ Base class for loss functions """
   sampler: BaseSampler
   def __init__(self, sampler: BaseSampler):
        super(Loss, self).__init__()
        self. sampler = sampler
   def value(self, xi: pt.Tensor, xi labels: Optional[pt.Tensor]):
        Perform forward pass.
       raise NotImplementedError("Please Implement this method")
```

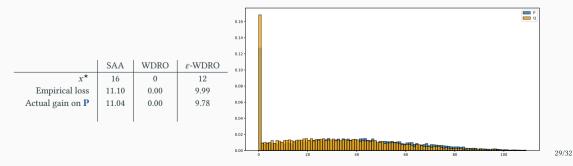
- ▷ A NewsVendor has to maximize its gain $-f_x(\xi) = -kx + u \min(x, \xi)$ by optimizing the number $x \in \mathbb{R}_+$ of newspaper bought, facing the uncertain demand of tomorrow
 - His buying price is k = 5 and his retail price is $u = 7 \rho = 2, \varepsilon = 0.1$
 - ♦ N = 20 i.i.d. samples from **P**
- ▷ Samples distribution P: "good day" $\mathcal{N}(50,5)$ w/ prob. 0.5, "bad day" $\mathcal{N}(20,5)$ w/ prob. 0.5, truncated at 0



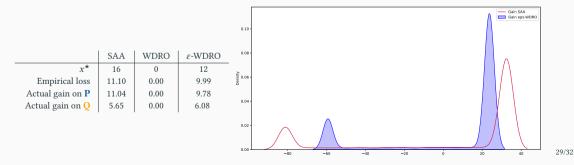
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- ▷ Samples distribution P: "good day" $\mathcal{N}(50,5)$ w/ prob. 0.5, "bad day" $\mathcal{N}(20,5)$ w/ prob. 0.5, truncated at 0
- ▷ Shifted distribution Q: "good day" $\mathcal{N}(50, 5)$ w/ prob. 0.3, "bad day" $\mathcal{N}(20, 5)$ w/ prob. 0.7, truncated at 0

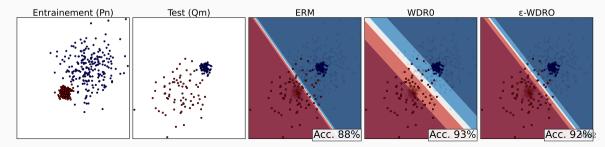


- ▶ A NewsVendor has to maximize its gain $-f_x(\xi) = -kx + u \min(x, \xi)$ by optimizing the number $x \in \mathbb{R}_+$ of newspaper bought, facing the uncertain demand of tomorrow
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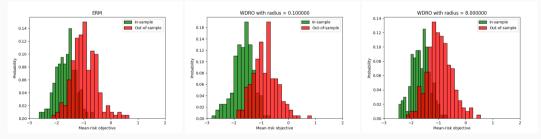
Back to example II – Logistic regression

- ▶ Regularization offers new possibilities:
 - ♦ Different transport costs squared norm, exotic ones
 - ♦ Regularization 11, 12, anything not data-driven
 - Scaling to larger datasets gradient-based methods instead of DCP
- ▶ Regularized WDRO as new robustness model:
 - ♦ ε is not necessarily small max(1 e^{-3} , ρ /10)
 - ♦ Absolutely continuous true distribution prior linked to transport cost



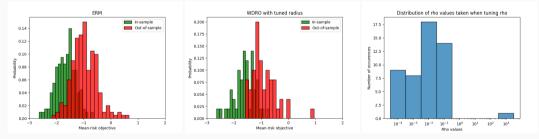
Back to example III - Portfolio selection

- ▶ 10 assets, N = 30, 200 simulations
- $\blacktriangleright \quad \text{Choice of the radius } \rho$
 - ♦ Cross validation inherited as a scikit-learn estimator
 - ♦ By statistically testing that the test distribution is encompassed



Back to example III - Portfolio selection

- ▶ 10 assets, N = 30, 200 simulations
- $\blacktriangleright \quad \text{Choice of the radius } \rho$
 - ♦ Cross validation inherited as a scikit-learn estimator
 - ♦ By statistically testing that the test distribution is encompassed



- ▶ Why optimizing correctly matters?
 - $\diamond\,$ Being accurate in λ enables to get a bound on the true risk
 - ♦ Instrumental to get the worst case distributions
- Toolbox underway!
 - ♦ Based on solving the dual regularized problem
 - ♦ AdamW using importance sampling for approximating the expectation
 - Default values for the radius, regularization, etc. from statistical study
- ▶ Currently undergoing testing on optimization and generalization
 - $\diamond~$ email me if you're interested in a $\beta\text{-version}$
- ▶ Paves the way to a widespread use of WDRO
 - ♦ Large class of objectives and costs not necessarily smooth
 - Cross validation of parameters

Conclusion



Hokusai

Fine Wind, Clear Morning (Gaifū kaisei) in Thirty-six Views of Mount Fuji (1830-1832)

Closing words

- ▶ Machine Learning models perform well but are they reliable?
 - ♦ Distributionally robust optimization provides an appealing framework to address this question
 - ◊ Interplay between statistics and optimization
- ▶ Wasserstein distributionally robust models are in!
 - ♦ Generalization and robustness guarantees
 - Widely implementable thanks to regularization
- ▷ Exciting perspectives: automated radius tuning, practical applications, robust feature selection, etc.



Azizian, I., Malick: *Regularization for Wasserstein Distributionally Robust Optimization*, arXiv 2205.08826, ESAIM: Control, Optimisation, and Calculus of Variations, 2023.

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Azizian, I., Malick: Exact Generalization Guarantees for (Regularized) Wasserstein Distributionally Robust Models, arXiv 2305.17076, NeurIPS, 2023.



Dapogny, I., Meda, Thibert. *Entropy-regularized Wasserstein distributionally robust shape and topology optimization*. ArXiv 2209.01500, Structural and Multidisciplinary Optimization, 2022.

Thank you! - www.iutzeler.org